

Supplementary Table 5-1. The performance of multi-label classification models trained on transcriptional profiles and molecular descriptors and fingerprints of drugs on the validation and the testing set. Cardiac dis S&S: MedDRA term for cardiac disorders signs and symptoms; dis: disorders. AUC: area under the receiver operating characteristic curve; Matthew correlation: MCC; CV: cardiovascular agents; CNS: central nervous system agents.

Antineoplastic agents						
	Cardiac dis S&S	Cardiac arrhythmias	Heart failures	Coronary artery dis	Pericardial dis	Myocardial dis
Accuracy	0.56	0.58	0.65	0.55	0.75	
Precision	0.61	0.46	0.50	0.66	0.02	
Recall	0.89	0.93	0.36	0.59	1	
F1 score	0.72	0.42	0.42	0.62	0.04	
AUC	0.60	0.63	0.76	0.35	0.95	
Kappa	0.00	0.26	0.18	0.06	0.03	
MCC	0.00	0.34	0.18	0.06	0.12	
Anti-inflammatory agents						
Accuracy	0.59	0.71	0.70	0.54		
Precision	0.35	0.00	0.00	0.11		

Recall	1.00	0.00	0.00	0.23		
F1 score	0.52	0.00	0.00	0.15		
AUC	0.86	0.78	0.76	0.57		
Kappa	0.28	0.00	0.00	0.00		
MCC	0.41	0.00	0.00	0.00		
CV						
Accuracy	0.62	0.68	0.87	0.54		
Precision	0.54	0.42	0.61	0.32		
Recall	0.88	0.90	1.00	0.98		
F1 score	0.67	0.57	0.76	0.49		
AUC	0.67	0.51	0.77	0.69		
Kappa	0.28	0.36	0.67	0.23		
MCC	0.32	0.43	0.72	0.35		
CNS						
Accuracy	0.58	0.59	0.74	0.57	0.96	0.90
Precision	0.42	0.38	0.22	0.43	0.00	0.00

Recall	0.70	0.66	0.28	0.58	0.00	0.00
F1 score	0.53	0.48	0.25	0.49	0.00	0.00
AUC	0.62	0.46	0.60	0.55	0.65	0.87
Kappa	0.20	0.18	0.10	0.12	0.00	0.00
MCC	0.22	0.20	0.10	0.13	0.00	0.00